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CONTROL OF CONTAMINANTS AROUND SPACECRAFT

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A high temperature octopole/collision cell apparatus (HT8P) was developed, along with the required cooling/power feedthroughs and modified "injector lens". The radio frequency operating characteristics of the HT8P were optimized, and the collision cell effective interaction length was determined in a series of calibration experiments. The well known $Ar^{+} + D^{2} \rightarrow ArD^{+} + D$ reaction was used in the calibration experiments, in which the HT8P was operated at temperatures up to 630 K (675°). The collision cell gas density versus temperature dependence for measurements with a capacitance manometer was modeled theoretically and verified experimentally using the same reaction. This dependence, due too thermal transpiration, provided additional evidence of the accuracy of the temperature measurement, which is a critical aspect in obtaining accurate cross sections for reactions of metal atoms.

The PL/GPID GIB instrument was used to continue the study of ion-molecule reactions that play a significant role in the low earth orbit spacecraft environment. One of the important reactions comprises collisions of atomic oxygen ions and water molecules. The extension of the study of these reactions to those with heavy water has been concluded.

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CONTROL OF CONTAMINANTS AROUND SPACECRAFT
1996 ANNUAL REPORT

The following report comprises a description of the activities performed in accordance with the contract between ORION International Technologies and the PL/GPID. Note that the Chemical Processes in the Space Environment Task of PL/WSSI, Spacecraft Interactions Branch, with which the contract was initiated, was transferred to PL/GPID during FY96.

1.0 ORIGINAL OBJECTIVES FOR YEAR 2

1. Complete the O^+ + Ba experiments using the GIB apparatus.

2. Design and construct a water cluster ion source for the GIB instrument. Install and determine the optimal conditions for producing water cluster ions of the sizes of interest.

3. Continue development of the fast neutral source in the HTMS.

4. Continue the ongoing program for studying the hyperthermal ion-molecule reactions involved in the spacecraft-ionosphere interactions using the GIB machine.

2.0 FORECAST FOR YEAR 2, AS PROPOSED AT THE END OF YEAR 1

1. Assemble and test the high temperature octopole/collision cell apparatus. The initial testing will be done in the HTMS, if possible. This stage would involve testing of the cell and octopole heating elements, and assessing the temperature at various locations of the device. The high temperature octopole/collision cell operating characteristics will be tested after installation in the GIB instrument. Testing will take place after the completion of a series of GIB water cluster ion experiments currently being carried out by PL/WSSI personnel.

2. Use the high temperature octopole/collision cell apparatus to determine the O^+ + Ba charge transfer cross section as a function of collision energy. This most important first stage may be followed up by attempting to elucidate the dynamics of the charge transfer process, through time-of-flight and emission studies.

3. Use the high temperature octopole/collision cell apparatus to study charge transfer reactions between important atmospheric ions, such as O^+, N^+, O_2^+, NO^+ and N_2^+, and other metals, such as Na and Mg, which have been observed in the ionosphere. In addition, the formation and chemistry of solvated metal clusters may be studied.

4. Use the GIB instrument, in its normal configuration, to continue the ongoing PL/WSSI program for studying hyperthermal ion-molecule reactions involved in the spacecraft-ionosphere interactions.

3.0 SUMMARY OF PROGRESS

1. The high temperature collision cell/octopole apparatus has been installed and calibrated. A manuscript, in which the apparatus is described and initial results are presented, has been submitted for publication in the Review of Scientific Instruments. An application for a patent of the high temperature apparatus has been initiated. The system is currently being used to study reactions of sodium with N_2^+, O_2^+, and NO^+.

2. Knudsen Cell experiments were conducted in the HTMS to confirm the sodium vapor pressure curve and to determine the purity of the sodium metal sample intended for use in the ion-metal atom studies. The HTMS has since been dismantled, in accordance with changing priorities at PL/GPID.

3. The $O^+ + H_2O/D_2O$ study carried out in GIB instrument was extended, on the advice of reviewers, prior to publication of the work in Chemical Physics Letters.

4. A new cluster ion source has been installed in the GIB instrument and the first experiments, on the photodissociation and collision-induced dissociation of $(N_2O{\bullet}H_2O)^+$ cluster ions, have been completed.

5. Work has been initiated on the design of a new bakeable GIB instrument which will incorporate the features of the HTMS and will eventually house the HT8P. The new instrument will feature provisions for more flexibility in experiment capabilities and *in situ* sample purity determinations.

4.0 TECHNICAL ACTIVITIES

4.1 ION-METAL ATOM CHARGE TRANSFER-GIB

The high temperature octopole/collision cell apparatus (HT8P) was installed in the GIB instrument, along with the required cooling/power feedthroughs and a modified "injector lens". The radio frequency operating characteristics of the HT8P were optimized, and the collision cell effective interaction length was determined in a series of calibration experiments. The well known $Ar^+ + D_2 \rightarrow ArD^+ + D$ reaction was used in the calibration experiments, in which the HT8P was operated at temperatures up to 630 K (675°F). The collision cell gas density versus temperature dependence for measurements with a capacitance manometer was modeled theoretically and verified experimentally using the same reaction. This dependence, due to thermal transpiration, provided additional evidence of the accuracy of the temperature measurement, which is a critical aspect in obtaining accurate cross sections for reactions of metal atoms.

Evaluation of the performance of the new octopole/injector arrangement indicated an improvement in ion beam energy distribution from a typical energy width of 0.30 eV, in the old system, to a spread of as low

as 0.12 eV. Prior to installation of the HT8P, the operating characteristics of the octopole rod heaters were tested in the vacuum environment of the HTMS instrument. In addition, the temperature versus heating power dependence of the HT8P pole heaters was determined *in situ* by spot welding a thermocouple directly to one of the poles, and monitoring the temperature as all the poles were heated. The thermocouple was subsequently removed to allow normal operation of the HT8P.

Because of limitations on operating temperature due to the proximity of the HT8P to low temperature materials in the GIB instrument, the first metal to be studied using the HT8P was sodium which required operation at moderate temperatures (~460 K). Studies of the charge transfer reactions of sodium with N_2^+, O_2^+, and NO^+ were undertaken and are nearly completed. The new data represent a significant improvement over existing data and will make an important contribution to the effort to model the behavior of atmospheric/ionospheric metal species derived via meteor ablation.

During the sodium metal work, modifications to the GIB instrument to accommodate operation of the HT8P at higher temperatures were designed and the necessary hardware was fabricated. The modifications primarily involved replacing Teflon insulators with assemblies manufactured of stainless steel and MACOR or of alumina. In addition, the vacuum system was fitted with turbomolecular pumps.

The sodium metal studies provided an excellent test case for evaluating the use of atomic absorption spectrometry (AAS) as an independent method for determining the density of metal vapor in the collision cell. For sodium, AAS and the temperature/vapor pressure results were in good agreement, although better reproducibility was obtained with the latter method. AAS was found to be accurate and will be important in studies of metals for which vapor pressure data are not of high quality.

In support of the planned HT8P study of the O^+ + Ba charge transfer cross section, additional experiments were done in the HTMS to improve our measurements of the Ba vapor pressure in the temperature range from 700 K to 900 K (427°C - 627°C). In addition, the measurement of barium vapor density using AAS was determined to be feasible, on the basis of the known spectroscopic characteristics of barium.

4.2 ION-MOLECULE REACTION STUDIES-GIB

The PL/GPID GIB instrument was used to continue the study of ion-molecule reactions that play a significant role in the low earth orbit spacecraft environment. One of the important reactions comprises collisions of atomic oxygen ions and water molecules. The extension of the study of these reactions to those with heavy water has been concluded. The isotope substitution was useful for elucidating aspects of the reaction dynamics for both the atom abstraction and charge transfer channels, and results from these experiments are included in publications 1 and 2, respectively, listed below. An attempt to extend the

isotopic substitution to include ^{18}O, on the advice of the reviewer for publication 1, failed to produce additional information.

4.3 CLUSTER ION STUDIES-GIB

The new cluster ion source, featuring a pulsed-supersonic nozzle crossed with a magnetically confined electron beam, was installed in the GIB instrument. Operation of the source was characterized, and optimal cluster formation conditions were determined. The system was first used to study $(N_2O \cdot H_2O)^+$ cluster ions in photodissociation and collision-induced dissociation experiments. This system was chosen since it had been studied previously. The new photodissociation experiments utilized the new PL/GPID YAG-pumped OPO laser. The design and characterization of this system was performed by PL/GPID personnel; the experiments included participation by ORION personnel. A publication (No. 4, below) of the results of this study is in preparation.

4.4 NEW INSTRUMENT DEVELOPMENT

The HTMS apparatus was disassembled and design work begun for a new high temperature (bakeable to 525 K) instrument. The new instrument incorporates the essential elements of the old HTMS, i.e., sensitive detection of neutral species, and will house the HT8P apparatus for GIB studies. The existing GIB instrument will be refitted with the original room temperature octopole/collision cell apparatus. The essential elements of the design necessary to perform GIB work were completed, and some electronic and vacuum components were ordered/received. Specifically, the designs of the main chamber, the coupling of the magnetic sector instrument to the main chamber, and the injection lens system are completed. Furthermore, vacuum feedthroughs, stainless steel components and flanges, Wien velocity filter chamber and electronics, and an arbitrary waveform generator have been ordered. The remaining design work includes the quadrupole mass spectrometer detection system, the details of the feedthrough flange assemblies, and if funds are available, a new electron impact ionization source. The remaining equipment ordering, including voltage power supplies and gas handling equipment, will be completed in the next fiscal year, pending funding.

In addition, we have proposed a second application of the new instrument involving the development of a fast neutral beam source. This application builds on the expertise gained from detailed studies of the translational energy dependence and disposal of ion-molecule reactions. We proposed studying the translational and internal energy dependence of chemical reaction cross sections of fast neutral-molecule reactions relevant to hypersonic flows. An important aspect of the new experiment is the generation of intense, mass selected positive-ion beams with well-defined kinetic energy distributions at energies between 1 and 20 eV. The generation of intense positive-ion beams is an existing capability in our laboratory, where 10 nA ion beam currents at ~10 eV are routinely achieved. The ion beam is then

converted to a neutral beam in a cell containing a charge-transfer target gas. As the previous studies of our laboratory have shown, charge transfer can readily provide 10% neutralization with minimal energy and momentum transfer, thus producing a neutral beam with high directionality and well-defined translational energy.

In the case of N_2 production, our laboratory studies have shown that the state-to-state dynamics of N_2^+ + H_2O charge-transfer collisions results in N_2 molecules that maintain the vibrational excitation of the parent ion. In addition, H_2O is an excellent charge-transfer target, because it can be efficiently pumped outside the cell, a necessity of this experiment. The neutral beam then passes through a second, thin cell containing a thermal target gas. The scattered and unscattered particles pass through an electron impact ionizer that is followed by efficient coupling of all ions to a quadrupole mass spectrometer for mass analysis and detection. Measurement of target gas density, primary neutral and secondary neutral intensities yield absolute cross sections. The design work to add these additional features is currently underway and will continue, pending funding for FY97 and PL/GPID priorities.

5.0 PATENT APPLICATION

A patent application entitled "High-Temperature Octopole Ion Guide with Coaxially Heated Rods", by Dale J. Levandier & Rainer A. Dressler, is currently awaiting processing at the Air Force ESC/JAZ office.

6.0 CONFERENCES ATTENDED

1. 1996 Air Force Office of Scientific Research Contractors' Review, Boulder, CO, 96 JUN 02 - 96 JUN 05.

2. The Gordon Research Conference on Atomic and Molecular Interactions, New London, NH, 96 JUN 30 - 96 JUL 05

3. The 14th International Symposium on Gas Kinetics, Leeds, UK, 96 SEP 07 - 96 SEP 12.

7.0 PRESENTATIONS

1. "High Temperature Guided-Ion Beam Experiment for Ion-Metal Vapor Collision Studies", Dale J. Levandier, Skip Williams, Rainer A. Dressler & Edmond Murad - a poster presented by Dale Levandier at the 1996 AFOSR Contractors' Review.

2. "Collision-Induced Dissociation and Photodissociation Studies of the $(N_2O{\cdot}H_2O)^+$ Cluster Ion", Michael J. Bastian, Rainer A. Dressler, Dale J. Levandier & Edmond Murad - a poster presented by Dale Levandier at the 14th International Symposium on Gas Kinetics.

8.0 PUBLICATIONS

1. A study of the isotope effects in the reaction $O^+ + H_2O/D_2O \rightarrow OH^+/OD^+ + OH/OD$ using guided-ion beams.

   Dale J. Levandier, Rainer A. Dressler & Edmond Murad

   Chemical Physics Letters, Vol. 251, pp. 174-181, 1996.

2. Empirical model of the state-to-state dynamics in near-resonant hyperthermal $X^+ + H_2O$ charge-transfer reactions.

   Rainer A. Dressler, Michael J. Bastian, Dale J. Levandier & Edmond Murad

   International Journal of Mass Spectrometry and Ion Processes, accepted for publication.

3. A high-temperature octopole ion guide for measuring absolute cross sections of ion-metal atom reactions.

   Dale J. Levandier, Rainer A. Dressler & Edmond Murad

   Review of Scientific Instruments, submitted for publication, 96 SEP.

4. Low energy collision-induced dissociation and photodissociation studies of the $(N_2O{\bullet}H_2O)^+$ cluster ion.

   Michael J. Bastian, Rainer A. Dressler, Dale J. Levandier, Edmond Murad, Felician Muntean & Peter B. Armentrout

   In preparation.

9.0 TRAINING

1. 96 MAY. Hazardous Waste Management Training - Refresher pursuant to EPA 40 CFR 260-279 (DL). The 4 hour course was conducted at Hanscom AFB by Institute for Environmental Education, Inc.

2. 96 MAY. Hazardous Waste Management Training - Initial pursuant to EPA 40 CFR 260-279 (SW). The 7 hour course was conducted at Hanscom AFB by Institute for Environmental Education, Inc.

10.0 FORECAST FOR YEAR 3

1. Conclude the HT8P-GIB study of sodium atom reactions.
2. Use the HT8P to determine the O^+ + Ba charge transfer cross section as a function of collision energy.
3. Use the HT8P to study charge transfer reactions between important atmospheric/ionospheric ions, such as O^+, N^+, O_2^+, NO^+ and N_2^+, and other metals, such as Mg and Ca, which have been observed in the ionosphere. In addition, the formation and chemistry of solvated metal cluster ions may be

studied. These species are expected to play important roles in metal transport phenomena in the upper atmosphere/ionosphere.

4. Use the GIB instrument, in its normal configuration or with the cluster ion source, to continue the ongoing PL/GPID program for studying hyperthermal ion-molecule reactions involved in the spacecraft-ionosphere interactions. These experiments will include photodissociation and collision-induced dissociation studies of excited molecular ion moieties of the sort generated in spacecraft thruster firings, and produced for the experiments in the supersonic nozzle cluster ion source. As a test case, we have proposed generating acetylene-water ion clusters in the cluster ion source. In the source region this moiety may undergo reactions producing isomeric structures, namely aldehyde and enol species, that can be distinguished in CID experiments.

5. Continue the development of the new GIB apparatus, including the design work on the fast neutral beam source.